

Safety Data Sheet

4-Nitrobiphenyl

Division of Safety
National Institutes
of Health



WARNING!

THIS COMPOUND IS ABSORBED THROUGH THE SKIN AND THE RESPIRATORY AND INTESTINAL TRACTS. IT IS CARCINOGENIC AND MUTAGENIC. AVOID FORMATION AND BREATHING OF AEROSOLS.

LABORATORY OPERATIONS SHOULD BE CONDUCTED IN A FUME HOOD, GLOVE BOX, OR VENTILATED CABINET.

AVOID SKIN CONTACT: IF EXPOSED, WASH WITH SOAP AND WATER.

FOR EYE EXPOSURE, IRRIGATE IMMEDIATELY WITH LARGE AMOUNTS OF WATER. FOR INGESTION, DRINK WATER, INDUCE VOMITING, OR REFER FOR GASTRIC LAVAGE. FOR INHALATION, REMOVE VICTIM PROMPTLY TO CLEAN AIR. ADMINISTER RESCUE BREATHING IF NECESSARY. REFER TO PHYSICIAN.

IN CASE OF LABORATORY SPILL, WEAR PROTECTIVE CLOTHING DURING CLEANUP. AVOID SKIN CONTACT OR BREATHING OF AEROSOLS. USE ETHANOL TO DISSOLVE COMPOUND. WASH DOWN AREA WITH SOAP AND WATER. DISPOSE OF WASTE SOLUTIONS AND MATERIALS APPROPRIATELY.

A. Background

4-Nitrobiphenyl (NBP) is a white to yellow crystalline solid and is stable at room temperature. It is moderately toxic to rats and rabbits and induces urinary bladder tumors in dogs when given orally. It is mutagenic in the Ames test. It has no commercial use and is used primarily in the laboratory as a model in cancer research.

B. Chemical and Physical Data

1. Chemical Abstract No.: 92-93-3

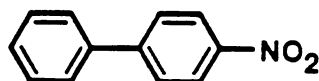
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• Synonyms:

NBP	p-Nitrodiphenyl
4-NBP	1-Nitro-4-phenyl benzene
PNB	4-Nitrodiphenyl
p-Nitrobiphenyl	4-Phenyl nitrobenzene
4-Nitro-1,1'-biphenyl (9CI)	

• Molecular
formula:
C12H9NO2

structure:



weight:
199.2

• Density: No data.

• Absorption spectroscopy: UV (isooctane): λ ($\log \epsilon$) = 295 (Weast, 1979); MS spectra have been reported (Meyerson et al 1966).

Volatility: No data.

Solubility: Very slightly soluble in water; slightly soluble in cold ethanol; soluble in benzene, chloroform, ether, acetic acid.

Description, appearance: White to yellow needle-like crystals.

Boiling point: 340°C.

Melting point: 113.8°C.

Stability: Stable at room temperature.

Chemical reactivity: Reduced to 4-aminobiphenyl by strong reducing agents. Oxidized by CrO₃ to 4-nitrobenzoic acid. Subject to ring substitutions like all aromatic compounds.

Flash point: No data.

Autoignition temperature: No data.

Explosive limits in air: No data.

Fire, Explosion, and Reactivity Hazard Data

NBP does not require special fire-fighting procedures or equipment and does not represent unusual fire and explosion hazards.

2. No conditions contributing to instability and no material incompatibilities are known.
3. No hazardous decomposition products are known.
4. NBP has a low vapor pressure and does not require nonspark equipment. When handled in flammable solvents, the precautions required for such solvents will apply.

Operational Procedures

The NIH Guidelines for the Laboratory Use of Chemical Carcinogens describe operational practices to be followed when potentially carcinogenic chemicals are used in NIH laboratories. The Guidelines should be consulted to identify the proper use conditions required and specific controls to be implemented during normal and complex operations or manipulations involving NBP.

1. Chemical inactivation: No validated method reported.
2. Decontamination: Turn off equipment that could be affected by NBP or the materials used for cleanup. Call the NIH Fire Department (dial 116) for assistance. Wipe off surfaces with ethanol, then wash with copious quantities of water. Glassware should be rinsed (in a hood) with ethanol, followed by soap and water. Animal cages should be washed with water.
3. Disposal: No waste streams containing NBP shall be disposed of in sinks or general refuse. Surplus NBP or chemical waste streams contaminated with NBP shall be handled as hazardous chemical waste and disposed of in accordance with the NIH chemical waste disposal system. Nonchemical waste (e.g., animal carcasses and bedding) containing NBP shall be handled and packaged for incineration in accordance with the NIH medical-pathological waste disposal system. Potentially infectious waste (e.g., tissue cultures) containing NBP shall be disinfected by heat using a standard autoclave treatment and packaged for incineration, as above. Burnable waste (e.g., absorbent bench top liners) minimally contaminated with NBP shall be handled as potentially infectious waste and packaged for incineration, as above. Absorbent materials (e.g., associated with spill cleanup) grossly contaminated shall be handled in accordance with the chemical waste disposal system. Radioactive waste containing NBP shall be handled in accordance with the NIH radioactive waste disposal system.
4. Storage: Store in screw-capped bottles with Teflon cap liners.

Monitoring and Measurement Procedures Including Direct Field Measurements and Sampling for Subsequent Laboratory Analysis

1. Sampling: Since NBP is used only under laboratory conditions, methods for field sampling and measurement have not been developed.

2. Separation and analysis: Direct analysis of NBP (preceded by separation if other nitro-compounds are present) has been carried out by polarography and by GC (Habboush and Norman, 1962). NBP may also be quantitatively reduced to 4-aminobiphenyl and determined colorimetrically (Koniacki and Linch, 1958).

Biological Effects (Animal and Human)

1. Absorption: NBP is absorbed into the animal and human body through the skin, by inhalation, and by ingestion.
2. Distribution: NBP is distributed to the liver in rats, monkeys and dogs.
3. Metabolism and excretion: The chief metabolic products of NBP are 4-nitrosobiphenyl and 4-aminobiphenyl; the latter is further oxidized to N-hydroxy-4-amino biphenyl. These three compounds, plus 4-amino-3-biphenylol hydrogen sulfate, have been identified as urinary excretion products (IARC, 1974).
4. Toxic effects: The oral LD50 is 2.23 g/kg in rats and 1.97 g/kg in rabbits. The target organs are red blood cells (production of methemoglobinemia, hemoglobinuria, and erythema) and the respiratory and intestinal tracts (irritation).
5. Carcinogenic effects: It is generally assumed that the carcinogenic action of NBP is due to its ready reduction in the animal body to 4-aminobiphenyl. Oral administration of NBP to dogs (900 mg per week over 33 months) produced urinary bladder tumors.
6. Mutagenic and teratogenic effects: NBP is a mutagen in the Ames test. There are no data concerning its teratogenicity.

Emergency Treatment

1. Skin and eye exposure: For skin exposure, remove contaminated clothing and wash skin with soap and water. For eye exposure, irrigate immediately with copious quantities of running water for at least 15 minutes. Consider ophthalmological consultation.
2. Ingestion: Drink plenty of water. Induce vomiting or refer for gastric lavage.
3. Inhalation: Remove victim promptly to clean air. Administer rescue breathing if necessary.
4. Refer to physician. Oxygen may be necessary during transport. Observe for methemoglobinemia.

References

Habboush, A.E., and R.O.C. Norman. 1962. The analysis of mixtures of isomeric benzenoid compounds by gas-liquid chromatography. J Chromatogr 7:438-446.

- IARC, International Agency for Research on Cancer. 1974. IARC Monographs the Evaluation of Carcinogenic Risk of Chemicals to Man. Some Aromatic Amines, Hydrazine and Related Substances, N-Nitroso Compounds and Miscellaneous Alkylating Agents, Vol. 4. World Health Organization, Geneva, Switzerland.
- Koniecki, W.B., and A.L. Linch. 1958. Determination of aromatic nitro compounds. Anal Chem 30:1134-1137.
- Melick, W.F., H.M. Escue, J.J. Naryka, R.A. Mezera, and E.P. Wheeler. 1955. The first reported cases of human bladder tumors due to a new carcinogen--xenylamine. J Urol 74:760-766.
- Meyerson, S., I. Puskas, and E.K. Fields. 1966. Organic ions in the gas phase. XVIII. Mass spectra of nitroarenes. J Am Chem Soc 88:4974.
- Weast, R.C., ed. 1979. Handbook of Chemistry and Physics, 60th ed. CRC Press, Cleveland, OH.